

# A Push-Button Molecular Switch

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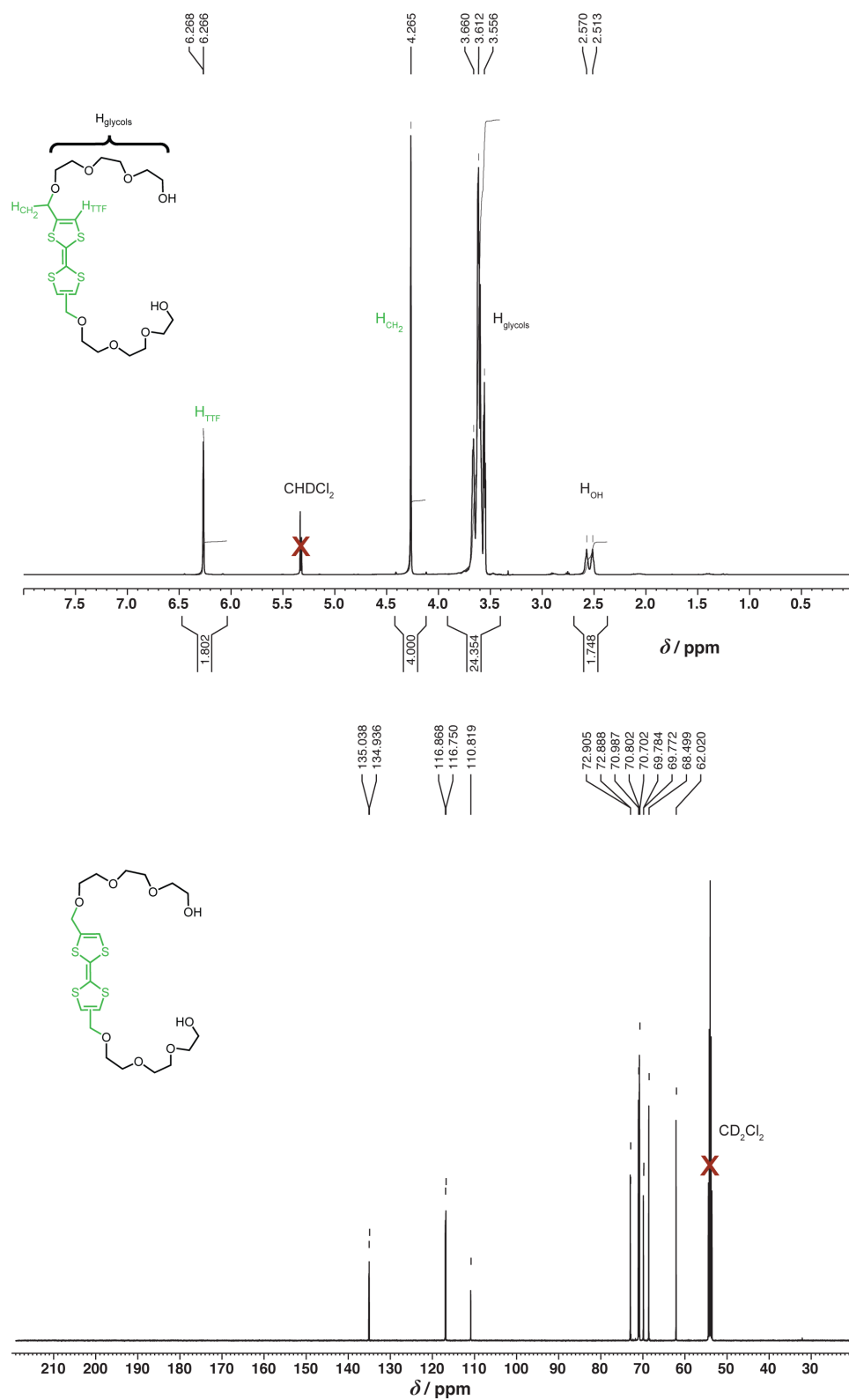
## Supporting Information

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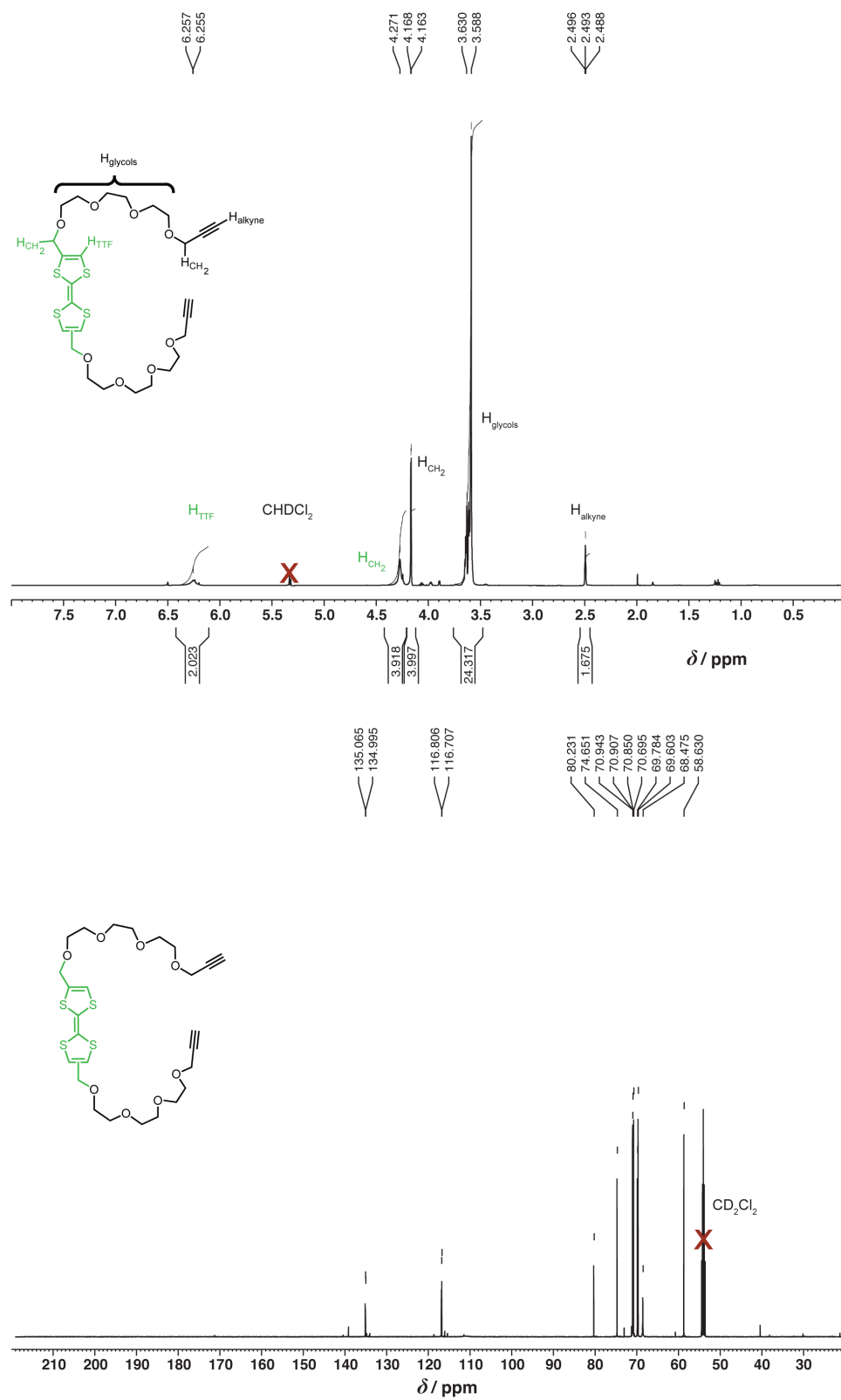
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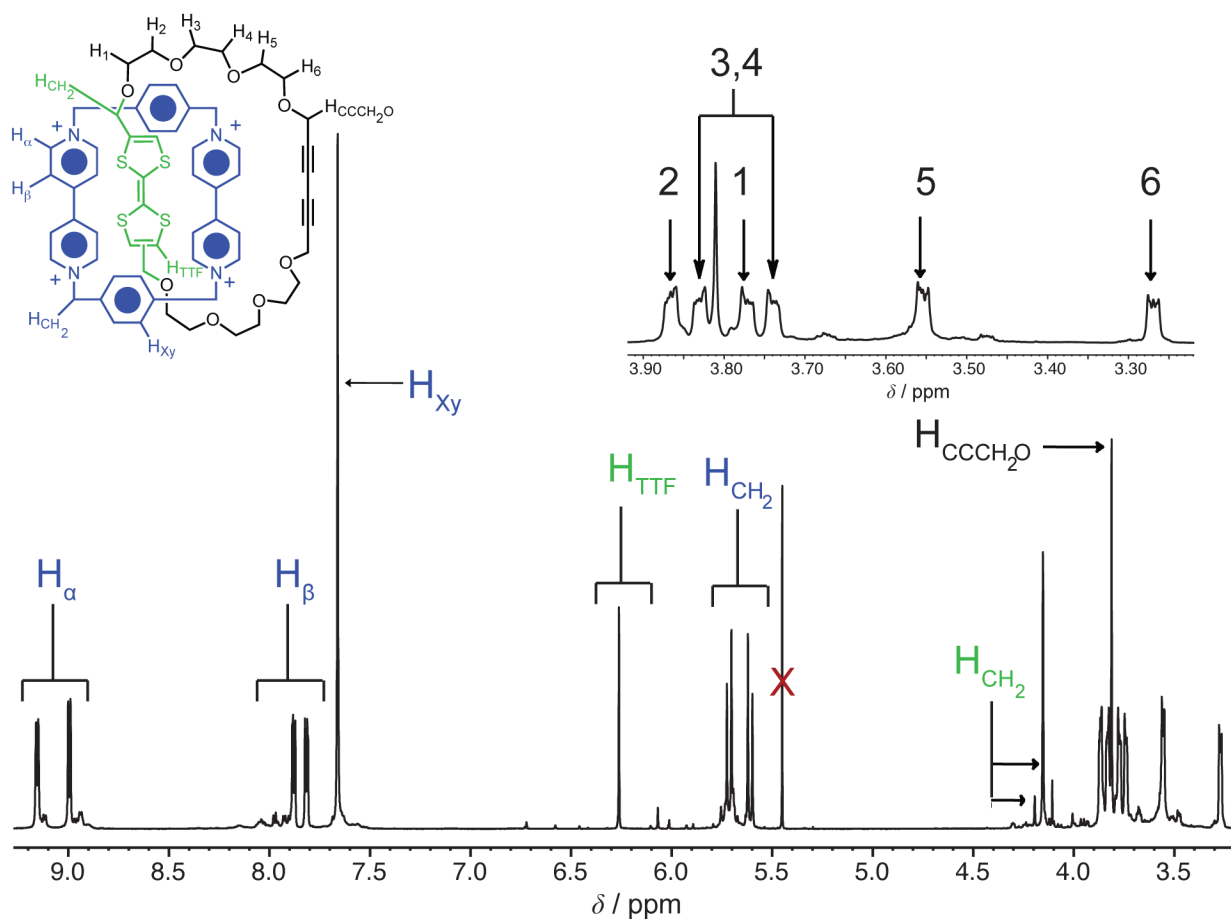
## Collection of 1D, 2D and VT NMR Spectroscopic Data



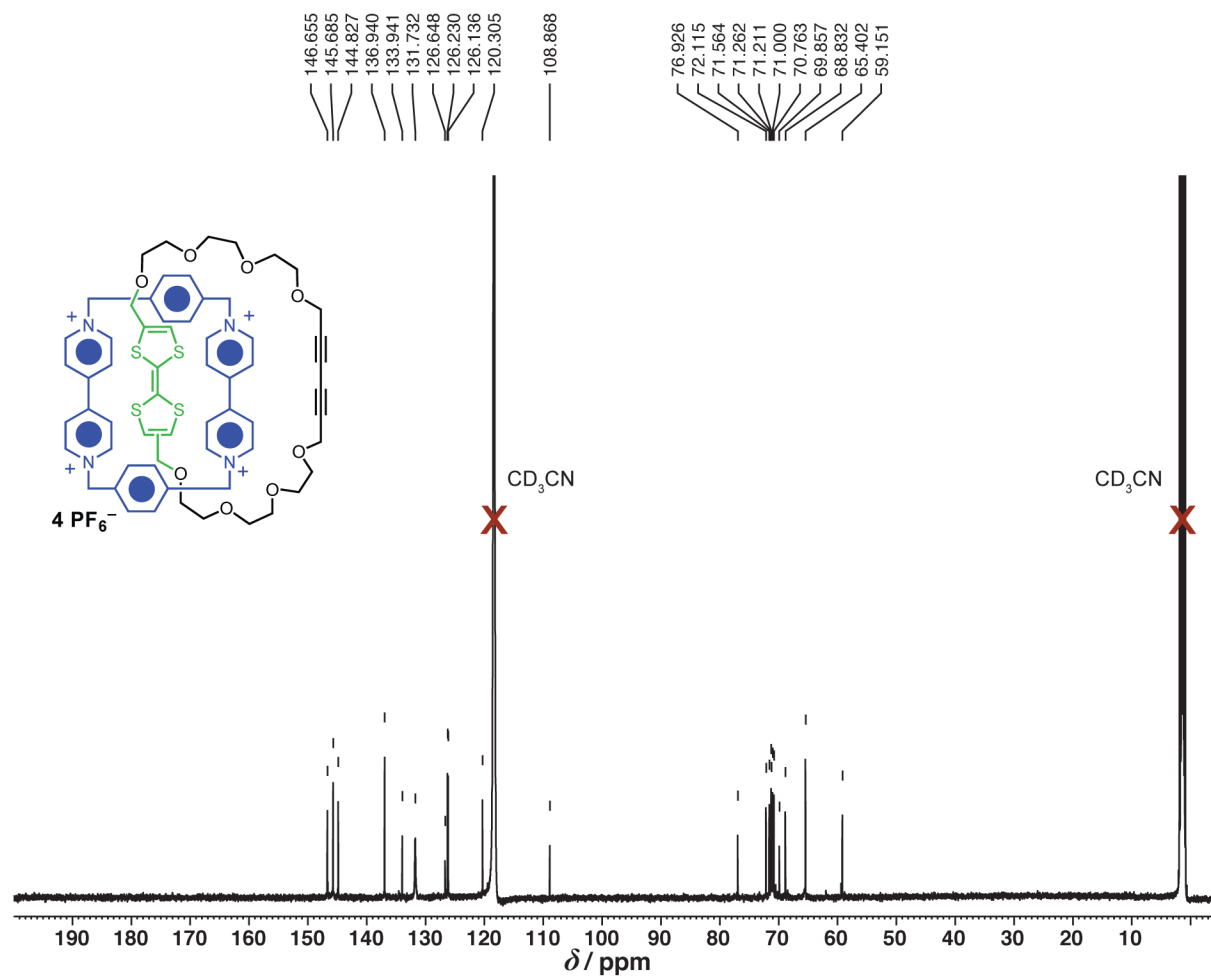
**Figure S1:** <sup>1</sup>H and <sup>13</sup>C NMR spectra of **3** (500 MHz; 125 MHz, 293 K, CD<sub>2</sub>Cl<sub>2</sub>)



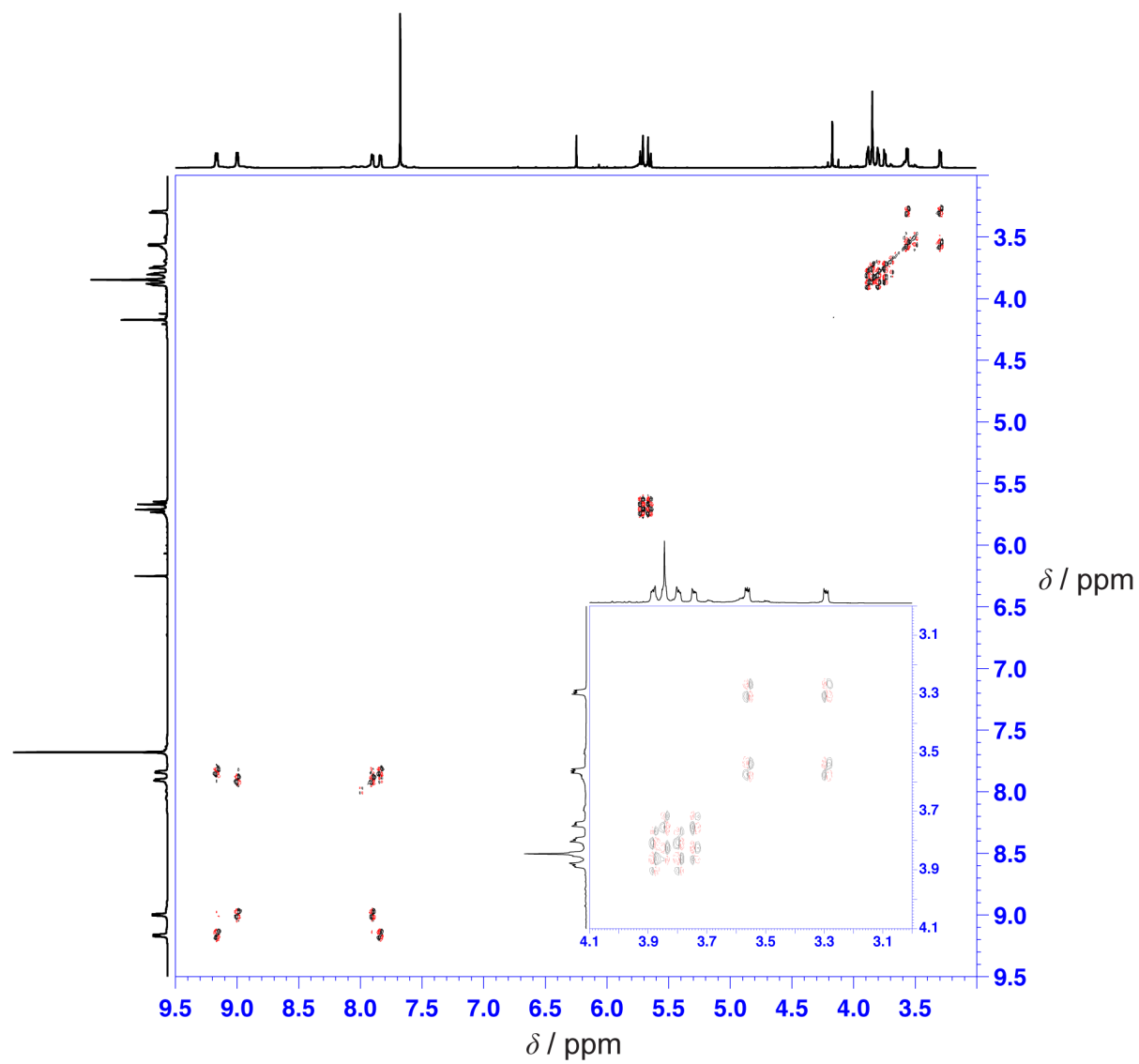
**Figure S2:**  $^1H$  and  $^{13}C$  NMR spectra of **4** (500 MHz; 125 MHz, 293 K,  $CD_2Cl_2$ )



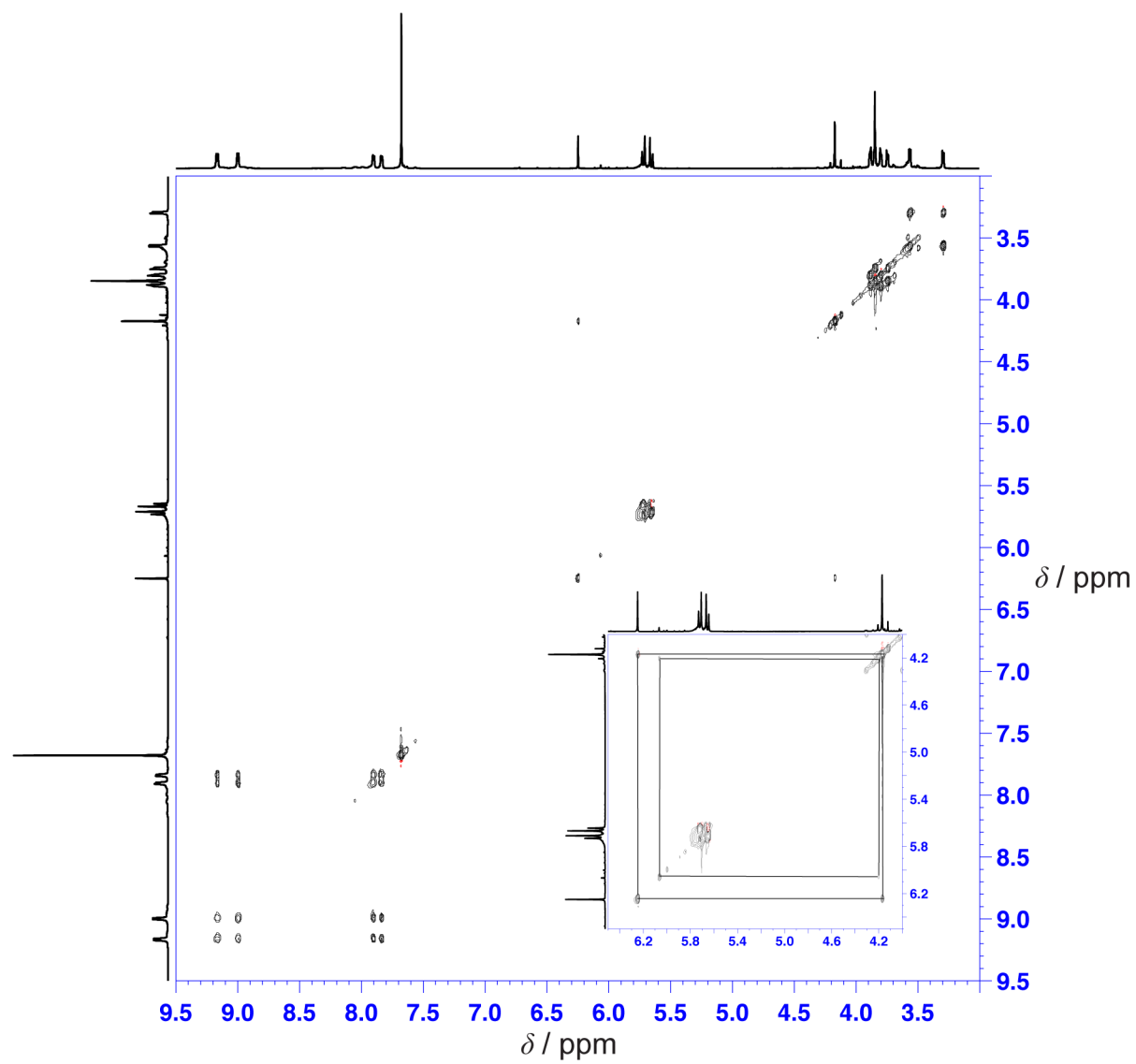
**Figure S3:** Fully annotated <sup>1</sup>H NMR spectrum of **1**·4PF<sub>6</sub> (500 MHz, 293 K, CD<sub>3</sub>CN)



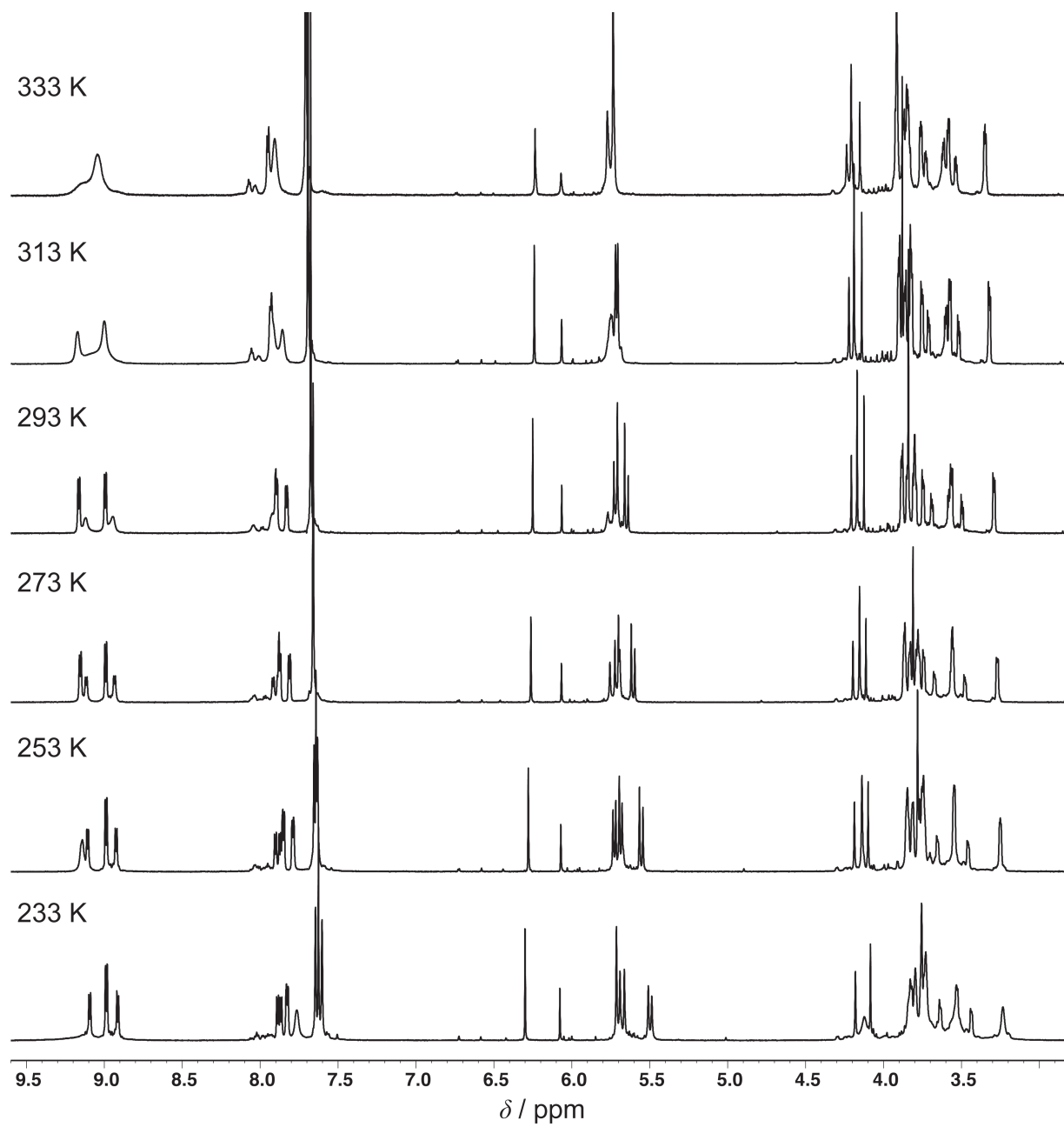
**Figure S4:**  $^{13}\text{C}$  NMR spectrum of **1**· $4\text{PF}_6$  (125 MHz, 293 K,  $\text{CD}_3\text{CN}$ )



**Figure S5:** COSY Spectrum of **1**·4PF<sub>6</sub> (600 MHz, 293 K)



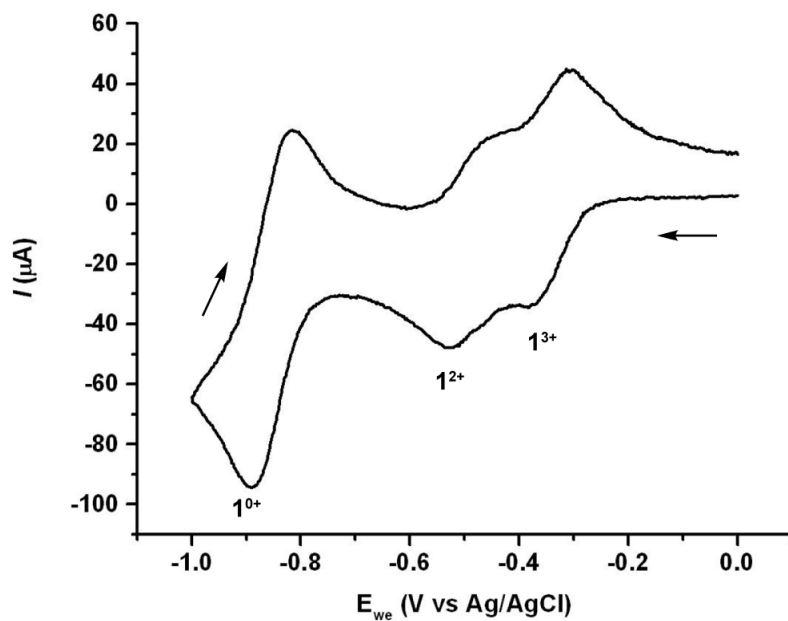
**Figure S6:** TOCSY Spectrum of **1**·4PF<sub>6</sub> (600 MHz, 293 K)



**Figure S7:** Variable Temperature  $^1\text{H}$  NMR spectra of  $1 \cdot 4\text{PF}_6$  (600 MHz)



## Additional Electrochemical Characterization



**Figure S8:** Reductive CV (200 mV/s) of  $1 \cdot 4\text{PF}_6$ ; reduction of  $1^{4+}$  displaying three reversible processes corresponding to the distinct first and second one electron reductions of the  $\text{CBPQT}^{4+}$  ring followed by the two electron process to the fully reduced, neutral  $\text{CBPQT}^{4+}$  ring.

## XYZ Coordinates for Calculated Structures

1·4PF<sub>6</sub> GSCC

N1	0.1257769724	-0.1159349357	-0.0708961535
C2	0.0957044104	-0.1119402762	1.2745020165
C3	1.2726130830	-0.1268357485	1.9947802425
C4	2.5021054036	-0.1738938441	1.3412487632
C5	2.4945380310	-0.2139346909	-0.0630960404
C6	1.3008747947	-0.1663402256	-0.7363704205
C7	3.7495791467	-0.1096525667	2.1110558215
C8	3.7603505780	-0.4403444664	3.4771482699
C9	4.9069463933	-0.2524545479	4.2065647992
N10	6.0272027331	0.2385802054	3.6344802877
C11	6.0620277797	0.5234636746	2.3192159043
C12	4.9425040167	0.3417935460	1.5369673054
C13	7.1844579309	0.6346428095	4.4782959445
C14	7.1033808844	2.0978987779	4.8165243668
C15	6.2883688970	2.5309517281	5.8646226696
C16	6.1070038569	3.8872325483	6.1052583338
C17	6.7658345755	4.8222472609	5.3078866660
C18	7.6341686683	4.3953088199	4.3080482897
C19	7.7800569569	3.0411242908	4.0418887924
C20	6.4223918720	6.2843131773	5.4090863351
N21	5.2915941745	6.5673169289	4.4736540698
C22	4.0364018300	6.2720381401	4.8748596177
C23	2.9905351088	6.3289761343	3.9847958718
C24	3.2146031158	6.6419923894	2.6343038513
C25	4.5372827907	6.9422670248	2.2569828756
C26	5.5489361641	6.9096089044	3.1906760616
C27	2.1193005006	6.5768503229	1.6654399940
C28	0.7720850747	6.5943642459	2.0880987052
C29	-0.2436022219	6.4315551099	1.1869224648
N30	0.0089587722	6.2460317715	-0.1337268918
C31	1.2851447255	6.2291936834	-0.5790730849
C32	2.3390432078	6.4241487934	0.2888663856
C33	-1.0993431532	5.8731865138	-1.0562709776
C34	-1.2980148724	4.3800748386	-1.0688176774
C35	-1.7964980410	3.7125857637	0.0542442010
C36	-1.8157364900	2.3286817043	0.0927972704
C37	-1.3294841842	1.5908138205	-0.9895338695
C38	-0.8993840011	2.2534585605	-2.1323927020
C39	-0.8934875438	3.6438976635	-2.1768304017
C40	-1.1356191793	0.1098866562	-0.8242568235
H41	-0.8807753064	-0.0891724757	1.7616927758
H42	1.1888678269	-0.0958790093	3.0759581541
H43	3.4137687801	-0.2671933370	-0.6387633898
H44	1.2396933932	-0.1448659668	-1.8203747714
H45	2.8871464537	-0.8558953998	3.9769862839
H46	4.9632210872	-0.4747213993	5.2676525861
H47	6.9886555847	0.9436518229	1.9296781913
H48	5.0075953384	0.6509629111	0.4966865707
H49	7.1463175638	-0.0035977458	5.3668349767
H50	8.0780708728	0.3664477896	3.9044908024
H51	5.7565200633	1.8122908212	6.4889269930
H52	5.4274382185	4.2085366998	6.8914550671
H53	8.1648425820	5.1184845990	3.7003743056
H54	8.3924816474	2.7276449680	3.1949476578
H55	7.2556375965	6.9254719293	5.1057743305
H56	6.0831385231	6.5630001477	6.4118017428
H57	3.8937783569	5.9636301373	5.9096736983
H58	2.0185354694	6.0418352695	4.3755475071
H59	4.8185847714	7.2068375553	1.2412820650
H60	6.5841499298	7.1280988271	2.9431291233
H61	0.5111385569	6.7510549761	3.1293464194

H62	-1.2885817525	6.4497774210	1.4797901396
H63	1.4376652550	6.0228748023	-1.6364405273
H64	3.3377913017	6.3706567742	-0.1377466956
H65	-0.8235737880	6.2383624056	-2.0500006916
H66	-1.9877015843	6.4164890015	-0.7143135812
H67	-2.1441176054	4.2674371719	0.9266492012
H68	-2.1633631581	1.8114154637	0.9865143736
H69	-0.5157077370	1.6999957643	-2.9894271386
H70	-0.5031070578	4.1491921096	-3.0545941235
H71	-1.9289718709	-0.3662643905	-0.2412358367
H72	-1.0455124182	-0.4152840245	-1.7807300134
O73	-1.7724215444	2.1106963843	3.3627833390
C74	-3.1366538705	1.8091923734	3.5631438968
C75	-3.4067853319	0.3355417327	3.7133835011
O76	-3.1310280696	-0.3155772468	2.4907553862
C77	-3.3734386896	-1.7030744714	2.6057627797
C78	-3.2009970241	-2.3527572220	1.2553989326
O79	-1.8478602370	-2.4795485216	0.8718618811
C80	-1.2260286122	-3.6538520661	1.3732165162
C81	0.1897836066	-3.3548692760	1.7739732926
O82	0.9610538152	-2.9720540465	0.6358732483
C83	2.0407091425	-3.8165473496	0.3477939585
C84	7.5261440993	-3.5411035660	4.1875221885
O85	8.1108187032	-2.2769580507	4.4055460032
C86	9.4302119245	-2.4121548361	4.8900164562
C87	10.0739972116	-1.0586344389	5.0344585946
O88	10.1880439879	-0.4857308274	3.7623733755
C89	10.6312243823	0.8490449153	3.7730494122
C90	10.6558453578	1.3479042355	2.3503750189
O91	9.3947414786	1.1381012221	1.7543688346
C92	9.3870371673	1.3689959363	0.3559650920
C93	8.7209808085	2.6650097579	-0.0211449261
O94	7.3236721879	2.5094185315	0.1666224245
C95	6.5788266122	3.4831983520	-0.5415174763
C96	5.1736596256	3.4445042712	-0.0503036741
C97	4.0858416197	3.2976868401	-0.8196352879
S98	2.5151388792	3.2717050393	-0.0493064270
C99	3.1764497782	3.3439066716	1.5792074858
S100	4.9098043169	3.6100521520	1.6908576025
C101	2.3753030408	3.1757127673	2.6807182091
S102	2.9878980062	3.0422655485	4.3168668212
C103	1.4413680056	2.5977529158	4.9994494240
C104	0.3739992649	2.5716483638	4.1927320510
S105	0.6349131045	3.0492068813	2.5153807544
C106	-1.0242683130	2.1845045924	4.5612086138
H107	-3.6722659981	2.1870618521	2.6818466877
H108	-3.5240468523	2.3457170320	4.4437235051
H109	-2.8044801067	-0.0995597091	4.5246778429
H110	-4.4717632842	0.1983447962	3.9782609550
H111	-4.4088575273	-1.8704629543	2.9558344631
H112	-2.6910470335	-2.1484441475	3.3509488032
H113	-3.6997779575	-3.3348270973	1.2495281108
H114	-3.7023243783	-1.7324014440	0.4982665580
H115	-1.2565590358	-4.4436149704	0.6013126418
H116	-1.7510058466	-4.0257598388	2.2670237350
H117	0.1887840674	-2.5389952775	2.4990554582
H118	0.6322910612	-4.2254788402	2.2792754417
H119	2.3513907311	-3.5920296573	-0.6830427097
H120	1.7342421336	-4.8787317288	0.3557214342
H121	7.3205332399	-4.0464945864	5.1498345055
H122	8.2299141739	-4.1962795531	3.6401356935
H123	10.0278859093	-3.0178332547	4.1869770992
H124	9.4377418643	-2.9300544789	5.8654677821
H125	9.4753987734	-0.4175332673	5.7073648562

H126	11.0632986542	-1.1811975247	5.5100466449
H127	11.6462610268	0.9326532414	4.1993813924
H128	9.9670515019	1.4730747761	4.3980663645
H129	10.9306494134	2.4183676634	2.3400502130
H130	11.4270207098	0.7936635103	1.7888494591
H131	8.8382691247	0.5396382941	-0.1127103377
H132	10.4139942000	1.3530017245	-0.0384335673
H133	9.1002665139	3.5091214461	0.5742680791
H134	8.9365348998	2.8836224309	-1.0809639209
H135	6.5803742916	3.2669308099	-1.6241094834
H136	7.0159201766	4.4795363134	-0.3987520880
H137	4.0947181412	3.2360174719	-1.9053768140
H138	1.4263586303	2.3845785649	6.0648174451
H139	-0.9990700986	1.2219605938	5.0915287190
H140	-1.4682238682	2.9375688572	5.2352558171
P141	2.3561853736	4.5751734091	-3.8706206647
F142	2.8552132203	5.5616193649	-5.0171773272
F143	3.1870066176	5.4192246496	-2.7390675022
F144	1.0567897339	5.5576072714	-3.5717095541
F145	1.4608047674	3.7252888454	-4.8995217114
F146	3.6247467341	3.5957207617	-4.0738651845
F147	1.8294117641	3.5876074104	-2.6580042545
P148	8.6670237965	6.4559314252	1.2065467233
F149	9.7651363197	7.5634300860	0.8799128384
F150	8.5549916595	7.0108759567	2.7572413652
F151	7.4603807731	7.4627414270	0.7922511081
F152	8.7311045251	5.8681301404	-0.2966568306
F153	9.8014322546	5.4000727691	1.6909715473
F154	7.5231236024	5.3262420807	1.5782280145
P155	-0.0658313536	-1.6476170842	5.2575014138
F156	-0.6517356943	-0.8673346725	3.9162820614
F157	0.7185519576	-0.2777754674	5.6453348849
F158	1.2487527104	-2.0887132886	4.3689989741
F159	-0.8330085278	-2.9837130782	4.7539143653
F160	-1.3712429788	-1.1567659770	6.0690079787
F161	0.5142516344	-2.3998179367	6.5373285883
P162	2.5270278959	4.4920595647	8.0028287439
F163	3.1231396396	3.8980590541	9.3616165994
F164	1.7543331055	5.6573126470	8.7778569897
F165	3.8521541044	5.4671627882	7.8420244630
F166	3.3414901403	3.3388162330	7.1481403662
F167	1.2460890404	3.5157495260	8.0678627692
F168	1.9779614324	5.0889130951	6.5660707804
C169	6.3007801395	-3.4469394402	3.4096842140
C170	5.2896207530	-3.4855218985	2.7407777513
C171	4.1654352334	-3.5554217250	1.9578636098
C172	3.1894684934	-3.6538618939	1.2427206240

#### 1-4PF<sub>6</sub> MSCC

N1	-0.5316580074	-0.1260882712	0.0683479090
C2	-0.4280580708	-0.0177883685	1.4060319883
C3	0.7979066410	-0.0310272373	2.0257266347
C4	1.9667018307	-0.0772496880	1.2562130967
C5	1.8206685020	-0.2126147542	-0.1288061400
C6	0.5739210244	-0.2457055768	-0.6949739030
C7	3.2897488471	0.1179036475	1.8664346540
C8	3.4285594098	0.2041762869	3.2547719518
C9	4.6372916128	0.5332717489	3.8126117150
N10	5.7164679650	0.7514075913	3.0310107625
C11	5.6286213876	0.6407025990	1.6902041127
C12	4.4324976859	0.3286474158	1.0850439302
C13	6.9593697089	1.3021380231	3.6294864619
C14	6.9446595019	2.8033577715	3.5533529616
C15	6.2357709715	3.5416124832	4.4976388732

C16	6.1450877592	4.9209469793	4.3778536637
C17	6.7542689142	5.5665969229	3.3044420923
C18	7.4670010773	4.8320488763	2.3545986832
C19	7.5629494364	3.4536766143	2.4835707586
C20	6.5169582442	7.0376055826	3.0932116208
N21	5.4259886061	7.1909332573	2.0862784645
C22	4.1607549815	6.9779331972	2.5011833026
C23	3.1450888772	6.8279349206	1.5830224639
C24	3.4511624944	6.8840631043	0.2233274313
C25	4.7529194896	7.1834593733	-0.1760845967
C26	5.7330792336	7.3250855288	0.7803460558
C27	2.4383836871	6.5345443022	-0.7854045142
C28	1.1307008169	7.0306544873	-0.7109856988
C29	0.1969086572	6.6001917257	-1.6201562548
N30	0.5167158718	5.6759102499	-2.5541237927
C31	1.7722854037	5.1945259640	-2.6579909564
C32	2.7631390241	5.6404531157	-1.8073909684
C33	-0.5644832470	5.0310720894	-3.3393315842
C34	-1.0345506227	3.7776651821	-2.6473433113
C35	-1.2656356525	3.7637317769	-1.2705568941
C36	-1.5980839978	2.5879767121	-0.6242645210
C37	-1.7206700160	1.4076149406	-1.3572490023
C38	-1.5355451643	1.4250176927	-2.7346841486
C39	-1.1843319646	2.6054133733	-3.3784705069
C40	-1.8345655053	0.1154937861	-0.6023139952
H41	-1.3473383859	0.1817463133	1.9459109910
H42	0.8066262083	0.0816671713	3.1072443155
H43	2.6646996460	-0.2507129452	-0.8064333161
H44	0.4420117383	-0.2848112720	-1.7714802653
H45	2.6028268869	0.0561979213	3.9394870302
H46	4.7435865593	0.6513821175	4.8872561033
H47	6.5110170432	0.8875580021	1.1031643264
H48	4.4012749208	0.3554209720	-0.0006778734
H49	7.0029419570	0.9427237963	4.6619243330
H50	7.8010904718	0.8725341819	3.0779392115
H51	5.7096151053	3.0549157856	5.3187127348
H52	5.5488693334	5.4799027839	5.0947421209
H53	7.9239202046	5.3252043317	1.4944455094
H54	8.0930683483	2.8778543039	1.7242453770
H55	7.3939068150	7.5595726624	2.6980302431
H56	6.1828904275	7.5301873013	4.0113045607
H57	3.9950211071	6.8967722379	3.5738317763
H58	2.1568635393	6.5883486269	1.9688880294
H59	5.0429690344	7.2611943517	-1.2185878069
H60	6.7705830300	7.4883313968	0.5031412426
H61	0.8485350823	7.7536199002	0.0483523231
H62	-0.8311047589	6.9496925758	-1.6214188261
H63	1.9435224750	4.4173948118	-3.3995230809
H64	3.7670224863	5.2331844280	-1.9130162377
H65	-0.1609267626	4.8010468542	-4.3304181711
H66	-1.3576342686	5.7784054167	-3.4621194669
H67	-1.1373384474	4.6631384720	-0.6706618073
H68	-1.7005384587	2.5726839918	0.4616305425
H69	-1.6070441486	0.5009443009	-3.3071355603
H70	-0.9705502913	2.5961004389	-4.4447120457
H71	-2.5924793256	0.1655954167	0.1860587130
H72	-2.0474129746	-0.7351625797	-1.2585508106
C73	0.7690729257	3.3109488413	3.1175532193
O74	-0.5032564592	2.8551932374	2.6694829435
C75	-1.3353732507	2.6276943489	3.7940955107
C76	-2.7636919005	2.5015815365	3.3318767845
O77	-2.9932850857	1.3680217465	2.5027490936
C78	-3.6838485649	0.2969517335	3.1121503754
C79	-2.8375474294	-0.4867338606	4.1002841888

O80	-3.4984569990	-1.7152056497	4.2847158710
C81	-2.8873792902	-2.5708152672	5.2196570574
C82	-1.5716688034	-3.1626149404	4.7512228959
O83	-0.5393354725	-2.1999411424	4.8170455255
O84	7.0297679430	-1.7703360611	-1.3043535164
C85	7.7589177130	-2.8836885445	-1.7702222972
C86	8.9321215556	-3.0792196544	-0.8293996764
O87	9.6521179932	-1.9031551817	-0.5771419808
C88	10.4072051575	-1.4293473943	-1.6693186944
C89	10.9557472114	-0.0568163196	-1.3333375493
O90	10.0744806706	0.9961532960	-1.6201293361
C91	8.9194796069	1.0393920394	-0.8185513663
C92	8.1423448872	2.2664235330	-1.2288926533
O93	6.9011447451	2.2237126720	-0.5450786104
C94	6.1118660444	3.3551373985	-0.8784512954
H95	1.1391676376	2.6841159040	3.9453643442
H96	0.6959685455	4.3243627624	3.5449576519
H97	-1.2647067326	3.4734420589	4.5009846262
H98	-0.9949719769	1.7367767213	4.3504147806
H99	-3.4312722269	2.4732090854	4.2070167253
H100	-3.0254276268	3.3908974691	2.7410882699
H101	-3.9765056413	-0.3889537916	2.3046211832
H102	-4.6131374910	0.6487838783	3.5885047749
H103	-1.8207582142	-0.6367724940	3.7054237965
H104	-2.7151349735	0.0450187762	5.0620846938
H105	-3.6020311461	-3.3852326730	5.3927997848
H106	-2.7186276437	-2.0496324316	6.1782016530
H107	-1.3300857403	-4.0317527255	5.3852459894
H108	-1.6869577408	-3.5290615413	3.7159664824
H109	8.0816105694	-2.7086408042	-2.8112852435
H110	7.1432987257	-3.8007976216	-1.7681644979
H111	8.5518544264	-3.4145846802	0.1439353668
H112	9.5846554562	-3.8769266244	-1.2301241832
H113	9.7937908060	-1.3329363237	-2.5816873204
H114	11.2308933928	-2.1324977455	-1.8912943783
H115	11.2544777367	-0.0507585480	-0.2690966942
H116	11.8513332122	0.1326206749	-1.9363477335
H117	9.1935587337	1.0858388636	0.2564371552
H118	8.2888629419	0.1461570885	-0.9495006912
H119	8.6852503278	3.1964253453	-0.9898997607
H120	7.9876569425	2.2613644571	-2.3200078138
H121	5.8605261882	3.3455593239	-1.9532425886
P122	2.7541726816	1.7350781683	-3.1746493361
F123	3.6019048905	1.2179411729	-4.4255464630
F124	3.6685443088	3.0771686622	-3.0778528145
F125	1.7165746058	2.5183135695	-4.1713673819
F126	1.8269180316	0.3937859499	-3.2417108477
F127	3.7779554428	0.9750714583	-2.1446623774
F128	1.8707861712	2.2573038032	-1.9090324011
P129	7.6707242040	6.5022159958	-2.3799368032
F130	9.1543876482	7.0939530392	-2.3337703314
F131	7.8022938228	6.0781408657	-0.7750664880
F132	7.0578927326	7.9349118678	-1.8759577260
F133	7.4816395359	6.9230205544	-3.9094189342
F134	8.2054698572	5.0382727909	-2.7802189423
F135	6.1272231152	5.9034168056	-2.3590065551
P136	1.7079091518	1.1269706139	6.4294995220
F137	0.5016436715	2.1793714342	6.4719540688
F138	2.5423014965	2.0749403675	5.4012334083
F139	0.9730810465	0.4146534594	5.0984961103
F140	0.8987832433	0.0887379475	7.3664723248
F141	2.4448167947	1.7735400015	7.6817772387
F142	2.9087093213	-0.0022590568	6.2712522309
P143	2.5649051641	5.6990171977	5.5505718826

F144	3.4475599533	4.7897551972	6.5345059295
F145	2.0103688635	6.5894718242	6.7570560197
F146	3.8569460221	6.7493506472	5.4069665509
F147	3.1613400438	4.8683533875	4.2681522006
F148	1.3102569714	4.7031632816	5.6401925363
F149	1.7607892288	6.6373366068	4.4626557453
C150	5.7636675633	-1.5981463507	-1.8860877278
H151	5.5320139006	-0.5246877326	-1.8178893895
H152	5.7591317671	-1.8579197026	-2.9573330046
C153	0.6600376780	-2.5802662402	5.4463014358
H154	0.4976479596	-3.4913501087	6.0468359692
C155	3.4835648444	-2.6983697788	-1.5365681606
C156	4.7234913428	-2.3907337720	-1.1421291961
S157	5.1732759697	-2.8459189838	0.5135700895
C158	3.5014395505	-3.1948135295	0.9913498593
S159	2.4077873869	-3.4776166895	-0.3729827603
C160	3.1182708718	-3.2248417321	2.2937653595
S161	4.2961359431	-3.0501703254	3.6038584943
C162	3.0770218965	-2.6463021200	4.8007091082
C163	1.7900352179	-2.8133561348	4.4848101384
S164	1.4416850306	-3.4081808995	2.8457161887
H165	3.0770716928	-2.4611327928	-2.5172093473
H166	0.9619164367	-1.7756204726	6.1299353378
H167	3.4090769525	-2.2357079979	5.7499119239
H168	6.6795298206	4.2824134915	-0.7033905760
C169	1.7704503758	3.3088711710	2.0714812609
C170	2.7406605147	3.3654805711	1.3425465865
C171	3.8710404413	3.3943016158	0.5704126773
C172	4.8908820090	3.3769430830	-0.0931960226